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APPLICATION OF A DISCRETE VELOCITY MODEL TO THE BOLTZMANN EQUATION IN SHEAR FLOWS

By James E. Broadwell

MAY 1963

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ABSTRACT

The application of a simple discrete velocity model to low Mach number Couette and Rayleigh flow is investigated. In the model, the molecular velocities are restricted to a finite set and in this study only eight equal speed velocities are allowed. The Boltzmann equation is reduced by this approximation to a set of coupled differential equations which are shown to be identical in form to those produced when the same approximation is applied to the Krook equation. The fluid velocity and shear stress in Couette flow are in approximate accord with those of Wang Chang and Uhlenbeck and of Lees over the complete range of Knudsen number.

INTRODUCTION

In a previous report (1), an approximate description of low Mach number rarefied shear flow was obtained by restricting the molecular velocities to a finite, prescribed set, an approximation which reduces the governing integro-differential equation to a set of coupled differential equations. That study was based on the Krook approximation to the Boltzmann equation and eight, equal magnitude, molecular velocities were allowed. It is the purpose of this report to show that when the same approximation is applied to the Boltzmann equation itself, the resulting set of differential equations is identical in form to that obtained from the Krook model; the only difference is in the magnitude of the relaxation time. In the Krook model this parameter was set equal to the mean time between collisions, $\lambda/\bar{c}$; here it is shown that it is approximately $\lambda/.68\,\bar{c}$. The Couette flow results of Ref. 1 are brought into approximate quantitative agreement with those of Wang Chang and Uhlenbeck (2) and of Lees (3) by the use of the new relaxation time. There is also significant improvement in the Rayleigh flow solutions.

THE DISCRETE VELOCITY MODEL

The Boltzmann equation may be written

$$\frac{\partial f}{\partial t} + u\frac{\partial f}{\partial x} + v\frac{\partial f}{\partial y} + w\frac{\partial f}{\partial z} = \left(\frac{\partial f}{\partial t}\right)_c = G - L \qquad (1)$$

in which f is the distribution function depending on the time and space variables t, x, y, z and on the molecular velocity $\vec{v}$ with components u, v, w.

The rate of change of f due to collisions is written as the gain minus the loss, G - L. Now if the molecules occupy, between collisions, a finite set of cells located at $\vec{v}_i$ in velocity space, Eq. (1) can be written

$$\frac{\partial N_i}{\partial t} + u_i \frac{\partial N_i}{\partial x} + v_i \frac{\partial N_i}{\partial y} + w_i \frac{\partial N_i}{\partial z} = \left(\frac{\partial N_i}{\partial t}\right)_c = G_i - L_i \qquad (2)$$

in which N_i is the number of molecules per unit volume with velocity $\vec{v}_i$.

Before evaluating $(G_i - L_i)$ for eight cells, consider as a simpler example the two - dimensional gas lying in the u, v plane with four velocities as sketched in Fig. 1a.

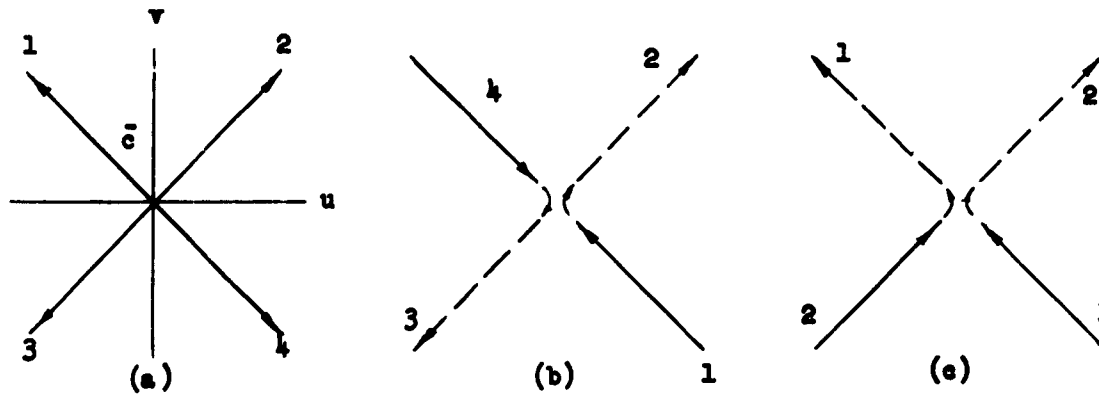

Figure 1

The speed is taken to be the mean thermal speed, $\bar{c}$. The rate of change of N_1, for instance, due to collisions is determined as follows. Loss of molecules from cell 1 occurs only when these molecules collide with those in cell 4, for collision with cell 2 or 3 occupants results only in an exchange of cells (see Figs. 1b and 1c). Thus the loss from cell 1 can be written

$$L_1 = v_r S_e N_1 N_4 = 2 \bar{c} S_e N_1 N_4$$

where v_r is the relative speed, equal to $2 \bar{c}$, and S_e is the effective collision cross section, i.e., the cross section which deflects collision partners from cells 1 and 4 to 2 and 3. These same arguments show, of course, that molecules are thrown into cell 1 from collisions 2 - 3; therefore

$$G_1 = 2 \bar{c} S_e N_2 N_3$$

and

$$\left(\frac{\partial N_1}{\partial t}\right)_c = 2 \bar{c} S_e (N_2 N_3 - N_1 N_4).$$

The expressions for the other cells can be written in the same way.

When there are eight cells, symmetrically placed in the eight velocity quadrants (see Fig. 2), and the flow is independent of z and symmetrical about the w = 0 plane,

$$N_1 = N_5, \; N_2 = N_6, \; N_3 = N_7, \; N_4 = N_8$$

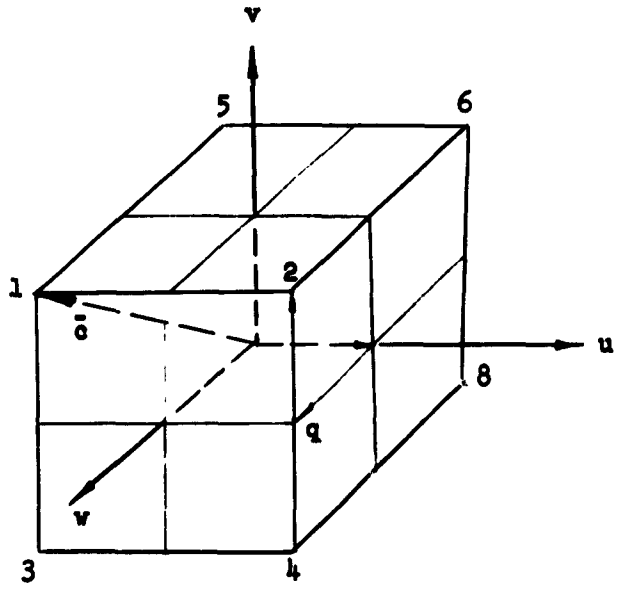

Figure 2

Under these conditions and with the assumption that the molecules are hard elastic spheres, it is shown in the Appendix that

$$\left(\frac{\partial N_1}{\partial t}\right)_c = \sqrt{2/3}\,(1 + 2/\sqrt{3})\,\bar{c}\,S\,(N_2\,N_3 - N_1\,N_4) \qquad (3)$$

where S is the mutual collision cross section.

Anticipating the application of these equations to low Mach number Couette and Rayleigh flow, let us divide Eq. (2) by the number density, N,

assumed constant. Then making use of Eq. (3) and corresponding expressions for the other cells we get,

$$\frac{\partial n_1}{\partial t} - q\frac{\partial n_1}{\partial x} + q\frac{\partial n_1}{\partial y} = 2\,\theta\,(n_2\,n_3 - n_1\,n_4) \tag{4a}$$

$$\frac{\partial n_2}{\partial t} + q\frac{\partial n_2}{\partial x} + q\frac{\partial n_2}{\partial y} = 2\,\theta\,(n_1\,n_4 - n_2\,n_3) \tag{4b}$$

$$\frac{\partial n_3}{\partial t} - q\frac{\partial n_3}{\partial x} - q\frac{\partial n_3}{\partial y} = 2\,\theta\,(n_1\,n_4 - n_2\,n_3) \tag{4c}$$

$$\frac{\partial n_4}{\partial t} + q\frac{\partial n_4}{\partial x} - q\frac{\partial n_4}{\partial y} = 2\,\theta\,(n_2\,n_3 - n_1\,n_4) \tag{4d}$$

where n_i is the fraction of molecules in cell i, $q = \bar{c}/\sqrt{3}$, and

$$\theta = \frac{1}{\sqrt{6}}\,(1 + 2/\sqrt{3})\,\bar{c}\,S\,N.$$

Several general features of these equations are worth noting. First, when they are multiplied successively by the collisional invariants, m, $m\,u_i$, $m\,v_i$ (m is the molecular weight) and summed, the right hand sides vanish, a consequence of the fact that the collisions sketched in Fig. 1 conserve the number of molecules and satisfy the equations of motion. (Energy is automatically conserved since the speed is constant.)

The equilibrium condition is

$$n_1\,n_4 = n_2\,n_3$$

a remnant of the general equilibrium condition

$$f(\vec{v}_1') \, f(\vec{v}_2') = f(\vec{v}_1) \, f(\vec{v}_2).$$

If the n_i 's are independent of x and y it is easy to show with the help of Eqs. (4) that the H function, defined by

$$H = \sum_i n_i \ln n_i,$$

obeys the equation

$$\frac{dH}{dt} = 2\theta \, (n_2 n_3 - n_1 n_4) \, (\ln n_1 n_4 - \ln n_2 n_3)$$

and hence

$$\frac{dH}{dt} \leq 0$$

as in the exact equation

COUETTE AND RAYLEIGH FLOW EQUATIONS

To apply Eqs. (4) to Couette and Rayleigh flow we assume, as was done in Ref. 1, that the fluid velocity in the y direction, V, is negligible (the walls are parallel to the x - axis) when the Mach number is low enough. Then since $V = \sum_i n_i v_i$,

$$n_1 + n_5 + n_2 + n_6 = n_3 + n_7 + n_4 + n_8 = \frac{1}{2}$$

and from the symmetry about w = 0,

$$n_1 + n_2 = n_3 + n_4 = \frac{1}{4}.$$

These relations make Eqs. (4b) and 4d), say, superfluous and allow the others to be written

$$\frac{\partial n_1}{\partial t} + q \frac{\partial n_1}{\partial y} = \frac{\theta}{2} (- n_1 + n_3) \tag{5a}$$

$$\frac{\partial n_3}{\partial t} - q \frac{\partial n_3}{\partial y} = - \frac{\theta}{2} (- n_1 + n_3) \tag{5b}$$

when the terms depending on x are dropped. These are Eqs. (18a) and (18c) of Ref. 1 with θ appearing in place of σ, quantities which differ only by a numerical factor.*

This is the result stated above, namely, that to the present approximation the Boltzmann and Krook equations lead to differential equations describing Couette and Rayleigh flow which are identical in form. This could perhaps be taken as simply an indication of the crudity of the eight cell model were it not for the many points of agreement, discussed in the following, between the results given by this simple model and those of much more rigorous analyses.

In the Krook model the magnitude of the effective collision rate must be chosen arbitrarily - it is of the order of the inverse of the mean time between collisions - and in Ref. 1 it was set equal to this quantity, i.e.,

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* In Ref. 1, n_1 represents the sum of the fraction of molecules in cells 1 and 5, i.e., 2 n_1; n_2 represents 2 n_2; etc. Eqs. (5), being linear, can be similarly interpreted.

to $\sigma = \bar{c}/\lambda$. It is shown in the Appendix that $\theta = .68\ \bar{c}/\lambda$. With this degree of arbitrariness removed from the discrete velocity model, it is worthwhile to compare the solutions, quantitatively, with those of Wang Chang and Uhlenbeck (2) and of Lees (3). Only Couette flow will be discussed here; the Rayleigh flow solutions, described in Ref. 1., are also improved when θ replaces σ but the details will be given in a later report.

COUETTE FLOW SOLUTION

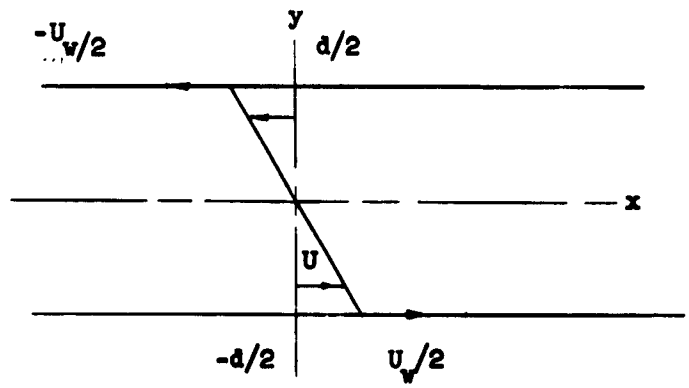

Figure 3.

Consider the steady Couette flow sketched in Fig. 3. For this problem Equations (5a) and (5b) can be written

$$\frac{d\, n_1}{d\, y^*} = \alpha(- n_1 + n_3) \tag{6a}$$

$$\frac{d\, n_3}{d\, y^*} = \alpha(- n_1 + n_3) \tag{6b}$$

where $y^* = y/d$ and $\alpha = d\ \theta/2\ q$

When the reflection from both walls is diffuse and $n_1 = n_5$, $n_2 = n_6$, etc., the boundary conditions are

$$\frac{q^2\left[- n_3(\tfrac{1}{2}) + n_4(\tfrac{1}{2})\right]}{q\ \left[n_3(\tfrac{1}{2}) + n_4(\tfrac{1}{2})\ \right]} = - \frac{U_w}{2}$$

$$\frac{q^2\left[- n_1(-\tfrac{1}{2}) + n_2(-\tfrac{1}{2})\right]}{q\ \left[n_1(-\tfrac{1}{2}) + n_2(-\tfrac{1}{2})\ \right]} = \frac{U_w}{2}$$

where U_w is the difference in the wall velocities. These equations state that the average x - component of velocity of the molecules leaving the upper wall is $- U_w/2$ at the upper wall and that of the upward flowing particles is $U_w/2$ at the lower wall. Then since $n_1 + n_2 = n_3 + n_4 = \frac{1}{4}$,

$$n_1(-\tfrac{1}{2}) = \tfrac{1}{8}(1 - U_w/2q),\ n_3(\tfrac{1}{2}) = \tfrac{1}{8}(1 + U_w/2q)$$

Solutions to Equations (6a) and (6b) satisfying these conditions are

$$n_1 = \frac{1}{8}\left[\frac{\alpha}{(\alpha+1)}\frac{U_w}{q}y^* + 1 - \frac{1}{2(\alpha+1)}\frac{U_w}{q}\right]$$

$$n_3 = \frac{1}{8}\left[\frac{\alpha}{(\alpha+1)}\frac{U_w}{q}y^* + 1 + \frac{1}{2(\alpha+1)}\frac{U_w}{q}\right]$$

From these 'distribution functions' the fluid velocity in the x direction, U, is found to be

$$U = \sum_i u_i n_i = 2q\left[-n_1 + n_2 - n_3 + n_4\right] = q\left[1 - 4(n_1 + n_3)\right]$$

$$= -\frac{\alpha}{(\alpha+1)}U_w y^* \qquad (7)$$

and the shear stress, p_{yx}, is given by

$$p_{yx} = \rho \sum_i u_i v_i n_i = 2\rho q^2\left[-n_1 + n_2 + n_3 - n_4\right] = 4\rho q^2\left[-n_1 + n_3\right]$$

$$= \frac{1}{2(\alpha+1)}\rho q U_w \qquad (8)$$

Defining the viscosity, μ, by $p_{yx} / \frac{dU}{dy}$ we have from Equations (7) and (8)

$$\mu = \rho q d/2\alpha = \rho q^2/\theta$$

and with $\theta = .68\,\bar{c}/\lambda$ and $q = \bar{c}/\sqrt{3}$,

$$\mu = .49\,\rho\,\bar{c}\,\lambda$$

compared with the classical value of $.499\,\rho\,\bar{c}\,\lambda$.

Next the fractional slip velocity, $2\,\Delta U/U_w$, defined by

$$2\,\Delta U/U_w = \frac{U_{w/2} - U_{(-\frac{1}{2})}}{U_w/2}$$

is, from Equation (7),

$$2\,\Delta U/U_w = \frac{1}{\alpha + 1} = \frac{1}{.59\,d/\lambda + 1} \qquad (9)$$

Lees finds, for Maxwell molecules,

$$2\,\Delta U/U_w = \frac{1}{.5\,d/\lambda + 1}$$

These expressions are shown in Figure 4, together with the results of Wang Chang and Uhlenbeck who also treated Maxwell molecules.

Finally, the ratio of the shear stress to the free molecule value, $p_{yx}/(p_{yx})_{f.m.}$, can be found from Equation (8) to be given, also, by

$$p_{yx}/(p_{yx})_{f.m.} = \frac{1}{\alpha + 1} = \frac{1}{.59\,d/\lambda + 1} \qquad (10)$$

Similarly, Lees' expression is

$$p_{yx}/(p_{yx})_{f.m.} = \frac{1}{.5\,d/\lambda + 1}$$

In Figure 4 the Wang Chang and Uhlenbeck values are compared with these two equations. Equation (10) lies below those of the other investigators at large d/λ because the value for the free molecule shear stress is given incorrectly by Equation (8) - it is approximately 15 percent too large. With this correction the shear stress is seen to be in good agreement with the Reference 2 value at large d/λ.

In summary, the simple discrete velocity model gives a reasonably accurate description of low Mach number Couette flow over the complete range of d/λ. It should be remembered, however, that the calculations of the collision cross sections in the Appendix can only be defended as being reasonable.

A further study of this flow with more molecular velocity cells is required before we can be sure that the accuracy of the eight cell solution is not simply fortuitous.

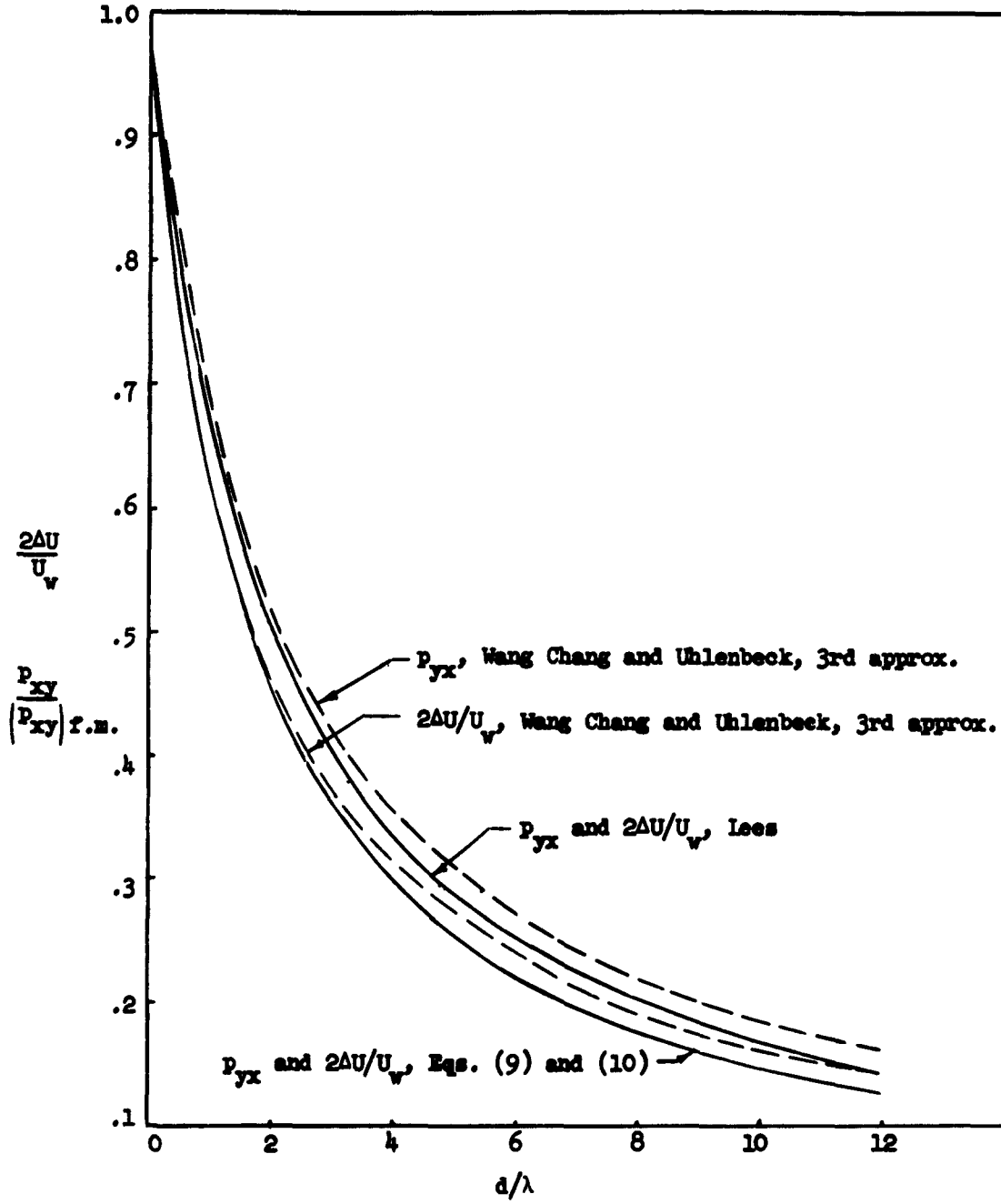

Figure 4.

Velocity slip and shear stress as a function of Knudsen number

APPENDIX

To find the rate of change of N_1 due to collisions we must first determine which of its possible collisions cause a net loss or gain from cell 1 as distinguished from those in which the collision partners simply exchange cells. Refer to Table 1 in which the sign of the velocity components are listed. Molecules may jump only between pairs of cells in which there is

cell	1	2	3	4	5	6	7	8
u	-	+	-	+	-	+	-	+
v	+	+	-	-	+	+	-	-
w	+	+	+	+	-	-	-	-

Table 1. Sign of velocity components

the same combination of signs for u, v, and w. Thus the collision 1-4 → 2-3 is possible but the collision 1-2 has no effect.

The collisions in which N_1 is depleted are:

$$1\text{-}4 \rightarrow 2\text{-}3 \qquad 1\text{-}6 \rightarrow 2\text{-}5 \qquad 1\text{-}7 \rightarrow 3\text{-}5$$

$$1\text{-}8 \rightarrow 2\text{-}7 \qquad 1\text{-}8 \rightarrow 3\text{-}6 \qquad 1\text{-}8 \rightarrow 4\text{-}5$$

and the rate of loss, L_1, is

$$L_1 = v_r^a \, s_e^a \, (N_1 N_4 + N_1 N_6 + N_1 N_7) + v_r^b \, s_e^b \, (N_1 N_8)$$

where the superscript a refers to the relative velocity and effective cross section of collision partners diagonally opposed on the faces of the velocity cube in Fig. 2 and b to those on the cube diagonals.

From symmetry, molecules from a collision 1-8, for instance, are equally distributed to 2-7, 3-6, and 4-5, and therefore the rate of addition to cell 1 is

$$G_1 = v_r^{\,a} s_e^{\,a}(N_2 N_3 + N_2 N_5 + N_3 N_5)$$

$$+ \frac{1}{3} v_r^{\,b} s_e^{\,b} (N_2 N_7 + N_3 N_6 + N_4 N_5)$$

The relative velocities are given by

$$v_r^{\,a} = 2\sqrt{\frac{2}{3}}\,\bar{c} \qquad v_r^{\,b} = 2\,\bar{c}.$$

The effective collision cross sections are determined for hard elastic spheres as follows. Consider first an encounter of the kind 1-4, which takes place in the w = constant plane, as sketched in Fig. 1b. The question is what fraction of those molecules that collide should be assigned to cells 2 and 3 (with the others being returned to 1 and 4). Since the scattering has circular symmetry the most reasonable assumption is that half of the colliding molecules are deflected, i.e., that

$$s_e^{\,a} = \tfrac{1}{2}\, s.$$

where s is the mutual collision cross section. The corresponding assumption for collisions such as 1-8, in which there is scattering in three dimensions, leads to the result

$$s_e^{\,b} = 1/\sqrt{2}\, s.$$

Finally, making use of the symmetry about $w = 0$, i.e., of the condition $N_1 = N_5$, $N_2 = N_6$, etc., and dividing G_1 and L_1 by N, we get

$$\left(\frac{\partial n_1}{\partial t}\right)_c = \frac{1}{N}(G_1 - L_1) = \sqrt{2/3}\,(1 + 2/\sqrt{3})\,\bar{c}\, SN(n_2\, n_3 - n_1\, n_4)$$

$$= 2\,\theta\,(n_2\, n_3 - n_1\, n_4)$$

where

$$\theta = \frac{1}{\sqrt{6}}\left(1 + \frac{2}{\sqrt{3}}\right)\bar{c}\, S\, N$$

The solutions of Eqs. (5a) and (5b) or Eqs. (18a) and (18c) of Ref. 1 and hence quantities such as viscosity, velocity slip, etc., are given directly in terms of θ but the fluid mechanical results are usually stated in terms of the mean free path, λ. To introduce this parameter we have to assume that the gas is close to equilibrium and that the velocity gradients are small, i.e., that in our case the N_i's are nearly equal.

The collision rate of all the molecules of cell 1, for instance, is given by

$$\varphi = \bar{c}\, S\left[2/\sqrt{3}\,(N_1\, N_2 + N_1\, N_3 + N_1\, N_5) + 2\sqrt{2/3}\,(N_1\, N_4 + N_1\, N_6 + N_1\, N_7) + 2\, N_1\, N_8\right]$$

$$= (6/\sqrt{3} + 6\sqrt{2/3} + 2)\,\bar{c}\, S\, N_1^{\,2} = 10.37\,\bar{c}\, S\, N_1^{\,2}$$

Then the collision frequency per molecule, σ, is

$$\sigma = \frac{\varphi}{N_1} = 10.37\ \bar{c}\ S\ N_1 = \frac{10.37}{8}\ S\ \bar{c}\ N = 1.3\ \bar{c}\ S\ N,$$

and

$$\lambda = \frac{\bar{c}}{\sigma} = \frac{1}{1.3\ SN}\ .$$

Now recall that

$$\theta = \frac{\pi}{\sqrt{6}}\ (1 + 2/\sqrt{3})\ \bar{c}\ S\ N = .88\ \bar{c}\ S\ N$$

and therefore

$$\theta = \frac{.88}{1.3}\ \sigma = .68\ \sigma = .68\ \frac{\bar{c}}{\lambda}\ .$$

SYMBOLS

$\bar{c}$	mean thermal speed
d	distance between walls in Couette flow
f	distribution function
G	gain in f due to collisions
H	Boltzmann H function
L	loss in f due to collisions
m	molecular weight
N	number of molecules per unit volume
N_i	number of molecules per unit volume with velocity $\vec{v}_i$
n_i	fraction of molecules per unit volume with velocity $\vec{v}_i$
p_{yx}	shear stress
$(p_{yx})_{f.m.}$	free molecule shear stress
q	$\bar{c}/\sqrt{3}$, component of $\bar{c}$ along coordinate axes
S	mutual collision cross section
S_e	effective collision cross section
t	time
U	x component of fluid velocity
U_w	difference in wall velocities
ΔU	velocity slip
u	x component of molecular velocity

SYMBOLS (Cont'd.)

V	y component of fluid velocity
v	y component of molecular velocity
$\vec{v}$	molecular velocity
v_r	relative molecular velocity
w	z component of molecular velocity
xyz	coordinate axes
y^*	y/d
α	d θ/2 q
θ	effective collision rate, $\frac{4}{\sqrt{6}} (1 + 2/\sqrt{3})\, \bar{c}\, S\, N = .68\, \bar{c}/\lambda$
φ	collision rate of occupants of one velocity cell, per unit volume
λ	mean free path
μ	viscosity
ρ	density, m N
σ	collision frequency per molecule , $\bar{c}/\lambda$

Superscripts

a	refers to collision partners on same face of velocity cube, Figure 2
b	refers to collision partners on velocity cube diagonals, Figure 2

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